

Lattice QCD+QED and isospin splittings

Kalman Szabo

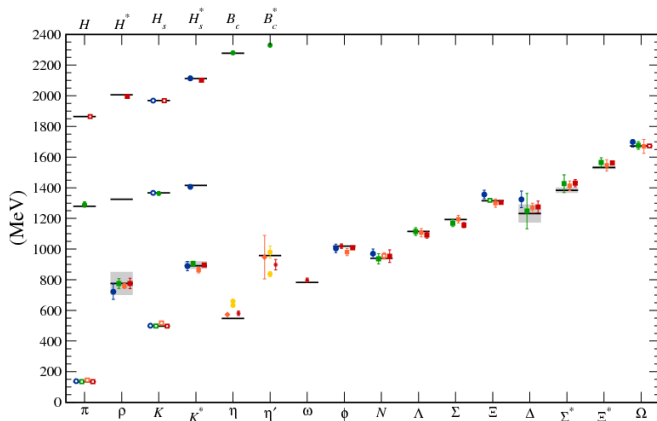
Forschungszentrum Jülich - Universität Wuppertal

Budapest-Marseille-Wuppertal collaboration:

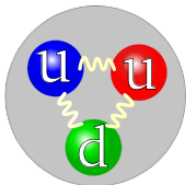
S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, L. Lellouch,
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Hadron spectrum from lattice QCD

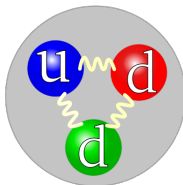
Several lattice QCD groups calculated the nucleon mass (and many more) to a few % accuracy. Compilation by [\[Kronfeld '13\]](#).



Proton

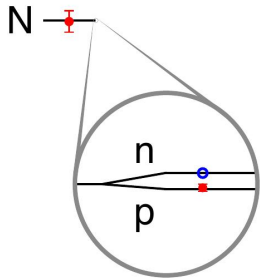


Neutron



SU(2) isospin symmetry: $u \leftrightarrow d$

Isospin symmetry



SU(2) is violated by

- quark mass difference
- electric charge difference

On the per mil level $\Delta M_N/M_N = 0.14\%$ arising from a competition of the two.

The value of ΔM_N is **necessary for the observed Universe:**

- $\delta M_N < 0.05\%$ \rightarrow inverse β -decay leaves only neutrons
- $\delta M_N > 0.14\%$ \rightarrow much faster β -decay, no heavy elements

arXiv:1406:4088

REPORT

NUCLEAR PHYSICS

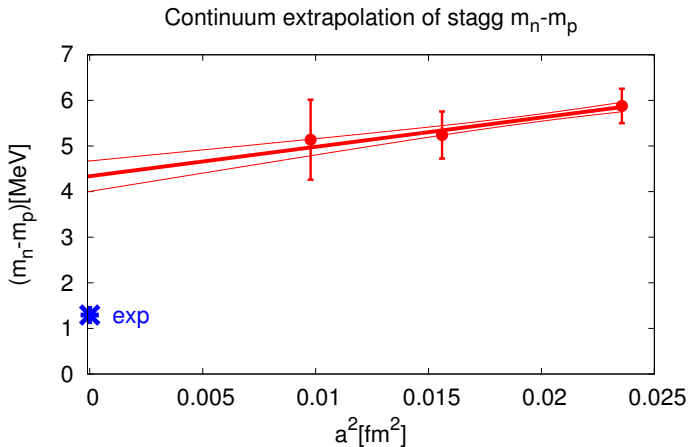
Ab initio calculation of the neutron-proton mass difference

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“It is difficult to get a grossly incorrect hadron spectrum.” [Hasenfratz, Montvay '82]

**It is easy to get a grossly incorrect
neutron-proton mass difference.**

$m_n - m_p$ with local staggered operators



Would need to project to taste singlet in valence.

→ **Use Wilson fermions instead.**

First full dynamical calculation of QCD+QED with non-degenerate u, d, s, c quarks.

All systematics on $m_n - m_p$ are taken into account upto $\mathcal{O}(\alpha^2)$.

Addressed **several issues in QED:**

- definition of finite volume QED
- finite volume corrections
- large noise/signal
- large autocorrelation

Challenging: **unprecedented precision** is required ($\times 1000$ more statistics for $m_n - m_p$ than for m_N)

Definition of QED in finite volume

Use non-compact formulation in Feynman-gauge:

$$2S = - \sum_x A_{\mu,x} \square A_{\mu,x} + \bar{\psi}_x \left(e^{iqA_{\mu,x}} \psi_{x+\mu} - e^{-iqA_{\mu,x-\mu}} \psi_{x-\mu} \right).$$

On periodic lattice **shift symmetry**, a remnant of gauge symmetry:

$$A_{\mu,x} \rightarrow A_{\mu,x} + c_\mu \quad \psi_x \rightarrow \exp(iqc_\mu x_\mu) \psi_x \quad \text{with} \quad c_\mu = \frac{2\pi}{L} n_\mu, n_\mu \in \mathbb{Z}$$

Eliminate, otherwise charged particle propagators will be zero:

- transform zero mode to $A_\mu(0) \in [-\pi/L, \pi/L]$ [Gockeler et al '92]
- remove zero mode $A_\mu(0) = 0$ [Duncan et al '96]
- C-periodic boundary condition [Wiese '91, Polley '95, Lucini et al '15]
- introduce photon mass [Endres et al '15]
- use infinite volume QED [Lehner '15]

Zero-mode subtraction

$$A_\mu(k=0) = 0$$

Removing zero mode does not change infinite volume physics.

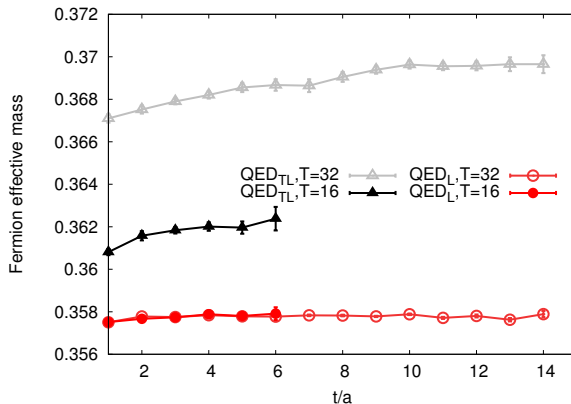
Many possible schemes, we study two choices:

- **QED_TL**: $A_\mu(k=0) = 0$ [Duncan et al '96]
- **QED_L**: $A_\mu(k_0, \vec{k}=0) = 0$ for all k_0 [Hayakawa, Uno '08]

Zero-mode subtraction

In **QED_TL masses are ill-defined** (used in previous studies).

No clear mass-plateaus, mass increases with T . It violates reflection positivity!



QED_L does not have these problems, T -independent masses.

Issues related to QED

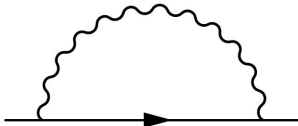
- definition of QED in finite volume
 - finite volume corrections
- dynamical QED: noise/signal problem
- dynamical QED: autocorrelation problem

Finite-volume effects in pure QED

Instead of the usual exponential [Luscher 85], the FV effects are **power like** ($1/L, \dots$). The FV effects are **large**, order of ΔM_N .

→ **Howto remove FV effects?**

What is the effect in a simpler case? Eg. pure QED:

$$\int \frac{dk_0}{(2\pi)} \left(\int \frac{d^3k}{(2\pi)^3} - \frac{1}{L^3} \sum_{\vec{k} \neq 0} \right) \times$$
A Feynman diagram showing a fermion line (solid line with an arrow) that forms a loop. A photon line (wavy line) is attached to the fermion line, forming a self-energy loop. The diagram is positioned to the right of the integral expression.

$$m(L)/m = 1 - \frac{\alpha \cdot 1.418\dots}{(mL)} - \frac{\alpha \cdot 2.837\dots}{(mL)^2} + \mathcal{O}\left(\frac{\alpha}{L^3}\right)$$

Finite volume effects in general

Proton is a **composite particle**, what are the FV effects?

- mesons in SU(3) PQ χ -PT [Hayakawa,Uno '08]
- meson/baryons in non-rel. eff. field theory [Davoudi,Savage '14]
- point particle in QED [BMWc '14]

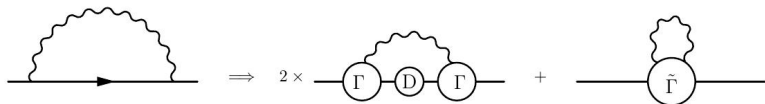
→ **same $1/L$ and $1/L^2$ behaviour**

$$m(T, L)/m = 1 - \frac{\alpha \cdot 1.418...}{(mL)} - \frac{\alpha \cdot 2.837...}{(mL)^2} + \mathcal{O}\left(\frac{\alpha}{L^3}\right)$$

The $1/L$ is a purely classical effect (static charge in a box).

Finite volume effects in general

Point particle propagator/vertex is replaced by dressed propagator and vertices (3pt and 4pt):



Finite volume effects can be calculated analytically:

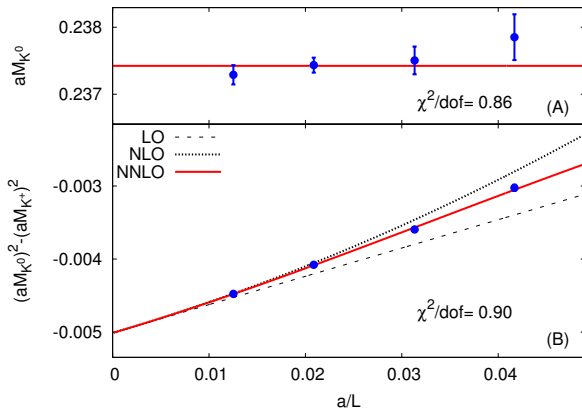
$$m(L)/m = 1 - \frac{\alpha \cdot 1.418\dots}{(mL)} - \frac{\alpha \cdot 2.837\dots}{(mL)^2} + \mathcal{O}\left(\frac{\alpha}{L^3}\right)$$

→ $1/L$ and $1/L^2$ are universal. (see also [\[Davoudi-Savage '14\]](#))

Large FV effects can be removed analytically!

FV dependence of the kaon mass

dedicated FV study: $L=2.5 \dots 8.0$ fm at the same parameters

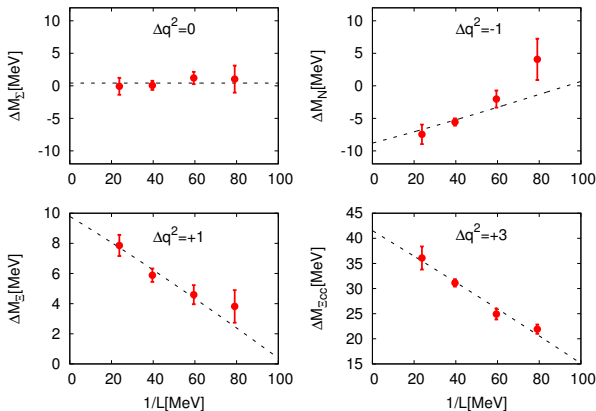


Neutral kaon shows no volume dependence.

Kaon splitting is perfectly described by formula with fitted $1/L^3$.

FV dependence of baryon masses

dedicated FV study: $L=2.5 \dots 8.0$ fm at the same parameters

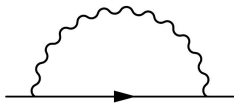


Σ splitting shows no volume dependence (cancels).

analysis strategy: include analytic corrections for the two universal orders and fit coefficient of $1/L^3$ (almost always insignificant)

Discrepancy in FV formula

Finite V effects in QED_L [BMWc '14]:



$$\frac{\Delta m}{m} = -\frac{\alpha\kappa}{2(mL)} - \frac{\alpha\kappa}{(mL)^2} + \frac{\alpha\pi}{(mL)^3} \times 3$$

Finite V effects in Non-Relativistic-QED [Davoudi,Savage '14]:

NRQED= low-energy effective field theory of QED



$$\frac{\Delta m}{m} = -\frac{\alpha\kappa}{2(mL)} - \frac{\alpha\kappa}{(mL)^2} + \frac{\alpha\pi}{(mL)^3} \times \frac{3}{2}$$

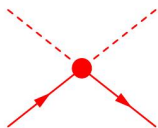
Discrepancy in FV formula

Finite V effects in NRQED [BMWc '15] [Lee,Tiburzi '15]

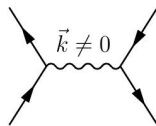
Missing graph: anti-fermion loop through a 4-fermion vertex.



There are no massless particles in the missing graph, so no power like FV behaviour is expected. But the vertex arises from a photon exchange:



has to be matched to



$$\frac{\Delta m}{m} = -\frac{\alpha\kappa}{2(mL)} - \frac{\alpha\kappa}{(mL)^2} + \frac{\alpha\pi}{(mL)^3} \times \left(\frac{3}{2} + \frac{3}{2} \right)$$

Discrepancy resolved by inclusion of anti-particles.

Issues related to QED

- definition of QED in finite volume
 - finite volume corrections
- dynamical QED: noise/signal problem
- dynamical QED: autocorrelation problem

Dynamical QED?

1. Do a perturbative-expansion: see [\[deDivitiis '13\]](#)

$$\Delta M_N(\alpha) = \Delta M_N(0) + \alpha \cdot \partial \Delta M_N(0) + \mathcal{O}(\alpha^2)$$

- complicated operators in $\partial \Delta M_N$
- disconnected diagramms (very difficult on large volumes)

2. Simulate dynamical QED:

- add photon field to the dynamics: simulate gluon+photon fields together
- no need to implement complicated/disconnected operators (let the computer do it for you)

Dynamical QED

Generate **gluon+photon** configurations simultaneously with a dynamical algorithm.

But there is a **noise/signal problem**:

$$\langle \Delta \rangle_e = e \cdot \text{noise} + e^2 \cdot \text{signal} + \dots$$

Simulate at **larger than physical** α , so signal outweighs noise:

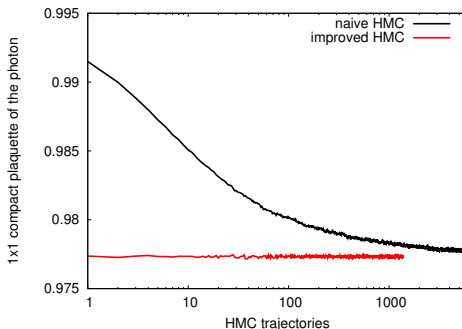
$$\frac{e^2}{4\pi} = \frac{1}{137} \longrightarrow \frac{1}{10}$$

Dynamical QED

long range QED \rightarrow **huge autocorrelation in standard HMC**

Solution: change kinetic term in HMC dynamics

$$\frac{1}{2} \sum_{x,\mu} P_{x,\mu}^2 \rightarrow \frac{1}{2} \sum_{x,\mu} P_{x,\mu} \square_{xy}^{-1} P_{y,\mu}$$



requires an FFT in every HMC step in the interacting case

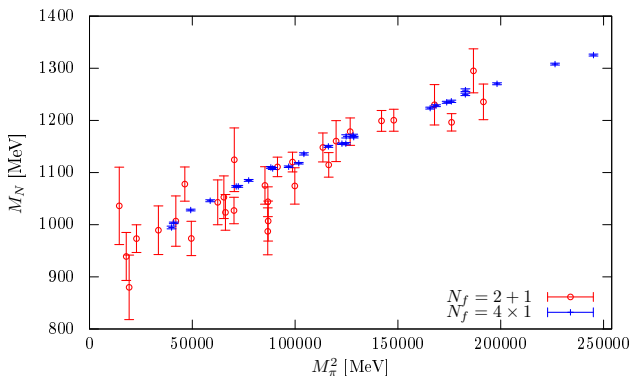
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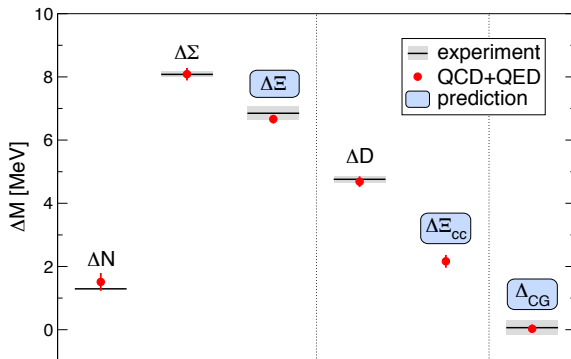
Simulations

About $1000\times$ more statistics for ΔM_N [BMWc '14] than for M_N [BMWc '08]. Recent algorithmic improvements:

- using 2-level multigrid inverter [Frommer et al '13]
- variance reduction technique [Blum,Izubuchi,Shintani '13]



Final results



- 5σ signal for neutron-proton mass difference
- three predictions + calculation of QCD/QED contributions
- $\Delta_{CG} = \Delta M_N - \Delta M_\Sigma + \Delta M_\Xi$ (Coleman-Glashow relation)
- full calculation - all systematics are estimated